ASYMPTOTIC BEHAVIOUR OF QUASI-ORTHOGONAL POLYNOMIALS

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8 April 2003

Abstract

We obtain explicit upper and lower bounds on the norms of the spectral projections of the non-self-adjoint harmonic oscillator. Some of our results apply to a variety of other families of orthogonal polynomials.

1 Introduction

We consider polynomials p_n which are orthogonal with respect to a complex weight σ on $[0,\infty)$ in the following sense. We suppose that p_n is of degree n and

$$\int_0^\infty p_m(x)p_n(x)\sigma(x)^2 \, \mathrm{d}x = \delta_{m,n}$$

for all non-negative integers m, n. (All of our statements and proofs can be rewritten with $(0,\infty)$ replaced by $\mathbf{R}$, and we will not keep repeating this point.) If $\sigma > 0$ and p_m are real-valued, then they are orthonormal in $L^2((0,\infty),\sigma(x)^2 \, \mathrm{d}x)$ in the usual sense, but for complex-valued σ such an interpretation is not possible. Our goal is to obtain bounds on the quantities

$$N_n = \int_0^\infty |p_n(x)\sigma(x)|^2 \, \mathrm{d}x$$

for all n.

This problem arose in the context of the non-self-adjoint harmonic oscillator

$$(Hf)(x) = -f''(x) + z^4x^2f(x) \tag{1}$$

acting in $L^2(\mathbf{R})$ for some complex z. In this situation the relevant weight is

$$\sigma(x) = \mathrm{e}^{-z^2x^2/2}$$

and N_n is the norm of the spectral projection P_n of H associated with its nth eigenvalue, $\lambda_n = z^2(2n+1)$. In the numerical literature N_n is called the condition number of the eigenvalue λ_n. Numerical calculations in [1] indicated that $\|P_n\|$ increases at an exponential rate as $n \to \infty$, and it was proved in [4] that there was no polynomial bound on $\|P_n\|$ for this and certain other Schrödinger operators. The super-polynomial rate of increase of the associated resolvent norms in the semi-classical limit was proved in [3] by a method which was greatly generalized in [6]. For certain classes of operators with analytic coefficients it was recently proved that the resolvent norms increase at an exponential rate in the semiclassical limit, [5]. However, the precise exponential constants have not been identified in any example.

A consequence of our theorems is that there exists a positive critical constant t_z such that the 'spectral expansion'

$$\mathrm{e}^{-Ht} = \sum_{n=0}^{\infty} \mathrm{e}^{-\lambda_n t} P_n$$

is norm convergent if $t > t_z$ and divergent if $0 \le t < t_z$. Our method provides explicit upper and lower bounds on t_z but not its precise value.

The problem may be reformulated as finding the norms of $\phi_n(x) = p_n(x)\sigma(x)$ in $L^2((0,\infty), \mathrm{d}x)$, where ϕ_n are obtained by applying a modified Gram-Schmidt orthogonalization process to the functions $x^n\sigma(x)$. This procedure is modified in the sense that we require

$$\int_0^\infty \phi_m(x)\phi_n(x)\ \mathrm{d}x = \delta_{m,n}$$

without any complex conjugates. This is equivalent to requiring that ϕ_m and $\phi_n^*(x) = \overline{\phi_n(x)}$ form a biorthogonal system in $L^2((0,\infty), \mathrm{d}x)$ in the sense that

$$\langle \phi_m, \phi_n^* \rangle = \delta_{m,n}$$

for all m, n. If P_n is the (non-orthogonal) projection

$$P_n f = \langle f, \phi_n^* \rangle \phi_n$$

then $P_m P_n = \delta_{m,n} P_n$ for all m, n and it is easily seen that

$$\|P_n\| = N_n.$$

In order to make some progress with this problem, we make the following assumptions on the weight σ. We assume that $\sigma(z)$ is an analytic function of z in the sector $S = \{z : |\arg(z)| < \alpha\}$, and that it is positive on the real axis. We also assume that

$$\int_0^\infty x^n |\sigma(\mathrm{e}^{i\theta}x)|^2\ \mathrm{d}x < \infty$$

for all $n \geq 0$ and $|\theta| < \alpha$, in order that p_n should be well-defined. Our most important condition is that

$$|\sigma(\mathrm{e}^{i\theta}r)| \geq c_\theta \sigma(s_\theta r) \tag{2}$$

for all $|\theta| < \alpha$ and all $r > 0$, where $c_\theta > 0$ and $0 < s_\theta < 1$. Our main theorem provides a lower bound on N_n for the weight $x \to \sigma(\mathrm{e}^{i\theta}x)$ under these assumptions. Examples of such weights are given in Section 3. Finally in Section 4 we compare the bounds obtained with numerical evidence.

2 The Lower Bound

Let $\{p_n\}_{n=0}^{\infty}$ denote the standard orthonormal sequence of real-valued polynomials with respect to the positive weight σ^2 on $(0, \infty)$. We define

$$p_{n,z}(x) = z^{1/2} p_n(zx)$$

where $z \in S$ and $x > 0$. If $z > 0$ then

$$\int_0^\infty p_{m,z}(x) p_{n,z}(x) \sigma(zx)^2 \, \mathrm{d}x = \delta_{m,n}$$

by making the change of variable $zx = u$. By analytic continuation the same holds for all complex $z \in S$. We are interested in obtaining a lower bound on the quantity

$$N_{n,z} = \int_0^\infty |p_{n,z}(x)\sigma(zx)|^2 \, \mathrm{d}x$$

for complex $z \in S$. Note that $N_{n,z} = 1$ for all positive real z.

Theorem 1 *Under the assumption (2) we have*

$$N_{n,z} \geq c_\theta^2 s_\theta^{-2n-1} \tag{3}$$

provided $z = r\mathrm{e}^{i\theta}$ and $|\theta| < \alpha$.

Proof We have

$$\begin{aligned} N_{n,z} &= |z| \int_0^\infty |p_n(zx)\sigma(zx)|^2 \, \mathrm{d}x \\ &\geq c_\theta^2 r \int_0^\infty |p_n(zx)\sigma(s_\theta r x)|^2 \, \mathrm{d}x \\ &= c_\theta^2 s_\theta^{-1} \int_0^\infty |p_n(zx/s_\theta r)\sigma(x)|^2 \, \mathrm{d}x. \end{aligned}$$

Now

$$p_n(zx/s_\theta r) = z^n s_\theta^{-n} r^{-n} p_n(x) + \sum_{j=0}^{n-1} k_j p_j(x)$$

for constants k_j which we need not evaluate. By the orthogonality of the polynomials, we have

$$\begin{aligned}\int_0^\infty |p_n(zx/s_\theta r)\sigma(x)|^2 \,\mathrm{d}x &= s_\theta^{-2n} + \sum_{j=0}^{n-1} |k_j|^2 \\ &\geq s_\theta^{-2n}.\end{aligned}$$

The statement of the theorem follows.

We next consider the example

$$\sigma(z) = z^{\gamma/2}\mathrm{e}^{-z^\beta}$$

where $\gamma > -1$ and $\beta > 0$. If $r > 0$ and $|\theta| < \pi/(2\beta)$ then

$$|\sigma(r\mathrm{e}^{i\theta})| = r^{\gamma/2}\mathrm{e}^{-r^\beta\cos(\theta\beta)} = c_\theta\sigma(s_\theta r) \tag{4}$$

where $s_\theta = \{\cos(\theta\beta)\}^{1/\beta}$ and $c_\theta = s_\theta^{-\gamma/2}$. After replacing $(0,\infty)$ by $(-\infty,\infty)$, the particular choice $\gamma = 0$ and $\beta = 2$ leads one to the study of the Hermite polynomials with a complex scaling, which is relevant to the non-self-adjoint harmonic oscillator. The choice $\beta = 1$ leads to the Laguerre polynomials L_n^γ. As far as we know, all other choices lead to non-classical polynomials.

The following theorem provides a more general type of weight satisfying (2), and can itself easily be generalized.

Theorem 2 *If*

$$\sigma(x) = \exp\{-\sum_{j=1}^n c_j x^j\}$$

for all $x \in (0,\infty)$, where $c_j \in \mathbf{R}$ for all j and $c_n > 0$, then σ satisfies (2) provided $|\theta| < \pi/(2n)$.

Proof We have to find $k_\theta > 0$ and $s_\theta \in (0,1)$ such that

$$\sum_{j=1}^n c_j\cos(j\theta)r^j \leq k_\theta + \sum_{j=1}^n c_j s_\theta^j r^j$$

for all $r > 0$ and $|\theta| < \pi/(2n)$. The validity of such an inequality depends upon the coefficient of r^n. We achieve the required bound $\cos(n\theta) < s_\theta^n < 1$ by putting

$$s_\theta = \{(1+\cos(n\theta))/2\}^{1/n}.$$

Note If $(0,\infty)$ is replaced by $\mathbf{R}$ in the above theorem, we must also assume that n is even.

3 The Upper Bound

It is surprisingly difficult to obtain an upper bound on N_n, and we treat only two cases. We start with the orthonormal sequence of Laguerre polynomials, associated with the weight $\sigma(x) = \mathrm{e}^{-x/2}$ on $(0, \infty)$. We have

$$\begin{aligned} p_n(x) &= \frac{(-1)^n}{n!} \mathrm{e}^x \frac{\mathrm{d}^n}{\mathrm{d}x^n} \left(x^n \mathrm{e}^{-x} \right) \\ &= \sum_{r=0}^{n} b_{n,r} x^r \end{aligned}$$

where

$$b_{n,r} = (-1)^{n-r} \frac{n!}{(r!)^2 (n-r)!}$$

satisfies

$$|b_{n,r}| \leq 2^n / r!$$

by virtue of the general inequality

$$(r+s)! \leq 2^{r+s} r!\, s!$$

The following theorem provides an upper bound on $N_{n,z}$ which complements the lower bound of Theorem 1.

Theorem 3 *If $\sigma(x) = \mathrm{e}^{-x/2}$ and $z = \mathrm{e}^{i\theta}$ then*

$$N_{n,z} \leq s_\theta^{-2n-1} 2^{4n+2}$$

for all $n \geq 0$, provided $|\theta| < \pi/2$ and $s_\theta = \cos(\theta)$.

Proof We start with the equality

$$N_{n,z} = s_\theta^{-1} \int_0^\infty |p_n(\mathrm{e}^{i\theta} x / s_\theta) \sigma(x)|^2 \, \mathrm{d}x,$$

which is proved as in Theorem 1. We have $c_\theta = 1$ and $s_\theta = \cos(\theta)$ by (4). We deduce that

$$\begin{aligned} N_{n,z} &\leq s_\theta^{-1} \int_0^\infty \sum_{r,s=0}^{n} |b_{n,r} b_{n,s}| s_\theta^{-r-s} x^{r+s} \mathrm{e}^{-x} \, \mathrm{d}x \\ &\leq s_\theta^{-2n-1} 2^{2n} \int_0^\infty \sum_{r,s=0}^{n} \frac{x^{r+s}}{r! s!} \mathrm{e}^{-x} \, \mathrm{d}x \\ &\leq s_\theta^{-2n-1} 2^{2n} \sum_{r,s=0}^{n} \frac{(r+s)!}{r!\, s!} \\ &\leq s_\theta^{-2n-1} 2^{2n} \left(\sum_{r=0}^{n} 2^r \right)^2 \\ &\leq s_\theta^{-2n-1} 2^{4n+2}. \end{aligned}$$

Note This proof can be extended to more general weights provided suitable bounds on the coefficients $b_{n,r}$ can be obtained, but in general this is not easy.

We next consider the non-self-adjoint harmonic oscillator. The orthonormal sequence of polynomials corresponding to the weight $\sigma(x) = \mathrm{e}^{-x^2/2}$ is given by $p_n(x) = k_n H_n(x)$, where

$$k_n = \pi^{-1/4} 2^{-n/2} (n!)^{-1/2}$$

and H_n are the Hermite polynomials

$$H_n(x) = (2x)^n - \frac{n!}{1!\,(n-2)!}(2x)^{n-2} + \frac{n!}{2!\,(n-4)!}(2x)^{n-4} - \ldots$$

We will need the following lemma.

Lemma 4 *If r, s are non-negative integers then*

$$\int_{-\infty}^{\infty} x^{2r+2s} \mathrm{e}^{-x^2}\ \mathrm{d}x \le \pi^{1/2} 2^{r+s} r!\, s!$$

Proof The left hand-side equals

$$\begin{aligned}\int_0^{\infty} u^{r+s} \mathrm{e}^{-s} s^{-1/2}\ \mathrm{d}s &= \Gamma(r+s+1/2)\\ &\le \pi^{1/2}\Gamma(r+s+1)\\ &\le \pi^{1/2} 2^{r+s} r!\, s!\end{aligned}$$

In the following theorem we restrict attention to the case of even integers; the treatment of odd integers is very similar.

Theorem 5 *Let $z = \mathrm{e}^{i\theta}$ where $|\theta| < \pi/4$, and put $s_\theta = (\cos(2\theta))^{1/2}$. Then*

$$N_{2n,z} \le \pi (n+1)^{1/2} 2^{4n+2} s_\theta^{-4n-1}.$$

for all non-negative integers n.

Proof We start with the identity

$$p_{2n}(x) = \sum_{r=0}^{n} b_{n,r} x^{2r}$$

where

$$b_{n,r} = \frac{(-1)^{n-r} 2^{2r-n} \sqrt{(2n)!}}{\pi^{1/4} (n-r)!\,(2r)!}.$$

In the following chain of inequalities we will use

$$2^{-2r}\sqrt{r+1} \le \frac{(r!)^2}{(2r)!} \le 2^{-2r}\sqrt{\pi(r+1)}$$

for all non-negative integers r; this is proved using induction and Stirling's formula.

Following the method of Theorem 3 we have

$$\begin{aligned}
N_{2n,z} &\leq s_\theta^{-1}\int_{-\infty}^{\infty}\sum_{r,s=0}^{n}|b_{n,r}b_{n,s}|s_\theta^{-2r-2s}x^{2r+2s}\mathrm{e}^{-x^2}\,\mathrm{d}x\\
&\leq s_\theta^{-4n-1}\sum_{r,s=0}^{n}|b_{n,r}b_{n,s}|\pi^{1/2}2^{r+s}r!\,s!\\
&\leq s_\theta^{-4n-1}2^{-2n}(2n)!\sum_{r,s=0}^{n}\frac{2^{3r+3s}r!\,s!}{(n-r)!\,(2r)!\,(n-s)!\,(2s)!}\\
&\leq s_\theta^{-4n-1}(n+1)^{-1/2}\left(\sum_{r=0}^{n}\frac{2^{3r}r!\,n!}{(n-r)!\,(2r)!}\right)^2\\
&\leq s_\theta^{-4n-1}(n+1)^{-1/2}\left(\sum_{r=0}^{n}2^{3r}\frac{n!}{(n-r)!\,r!}\frac{(r!)^2}{(2r)!}\right)^2\\
&\leq s_\theta^{-4n-1}(n+1)^{-1/2}2^{2n}\left(\sum_{r=0}^{n}2^{3r}\frac{(r!)^2}{(2r)!}\right)^2\\
&\leq s_\theta^{-4n-1}(n+1)^{-1/2}2^{2n}\left(\sum_{r=0}^{n}2^{r}\sqrt{\pi(r+1)}\right)^2\\
&\leq s_\theta^{-4n-1}\pi(n+1)^{1/2}2^{4n+2}.
\end{aligned}$$

4 The Spectral Expansion

Let H denote the non-self-adjoint harmonic oscillator acting in $L^2(\mathbf{R})$, with eigenvalues $\lambda_n = z^2(2n+1)$ and spectral projections P_n. If the right hand-side of the expansion

$$\mathrm{e}^{-Ht} = \sum_{n=0}^{\infty}\mathrm{e}^{-\lambda_n t}P_n \tag{5}$$

is norm convergent, then by comparing the action of the two sides on the eigenfunctions ϕ_n we see that they coincide on a dense subspace, and hence on the whole of $L^2(\mathbf{R})$.

If we put

$$s_z = \limsup_{n\to\infty} n^{-1}\log(\|P_n\|)$$

then our theorems imply that $0 < s_z < \infty$ provided $0 < |\theta| < \pi/4$. They also provide explicit upper and lower bounds on s_z.

Theorem 6 *The spectral expansion (5) is norm convergent if* $t > t_z = s_z/(2\cos(2\theta))$ *and is norm divergent if* $0 \leq t < t_z$.

Proof For $t > t_z$ the terms of the series decrease at an exponential rate, while for $0 \leq t < t_z$ they are not uniformly bounded in norm.

5 Numerical Results

The non-self-adjoint harmonic oscillator (1) has eigenvalues $\lambda_n = z^2(2n+1)$ and eigenfunctions

$$\phi_n(x) = k_n \mathrm{e}^{-z^2x^2/2} H_n(zx)$$

for $n = 0, 1, ...$, where k_n are normalization constants, H_n are the Hermite polynomials, and $|\arg(z)| < \pi/4$.

Theorem 7 *If P_n is the* nth *spectral projection of H and $z = r\mathrm{e}^{i\theta}$ then*

$$\liminf_{n\to\infty} n^{-1} \log(\|P_n\|) \geq \log(\sec(2\theta)).$$

Proof This follows directly from Theorem 1 upon observing that $\|P_n\| = N_{n,z}$ and $s_\theta = \cos(2\theta)^{1/2}$.

We have previously evaluated these norms numerically for $z^4 = c = \sqrt{i}$, i.e. $\theta = \pi/16$. See $\kappa_n^{(1)}$ in Table 4 of [1]. It appears from the computations there that

$$\lim_{n\to\infty} n^{-1} \log(\|P_n\|) \sim 0.40$$

which is considerably larger than the lower bound 0.079 of Theorem 7.

We now report on a more systematic numerical investigation of the spectral projections of (1). We evaluated $\sigma_n(\theta) = \sqrt{\|P_n\| / \|P_{n-2}\|}$ for various n and θ using Maple. (This was easier than evaluating $\|P_n\| / \|P_{n-1}\|$ because different algorithms are needed for even and odd n.) The method used was the same as that described in [1, sect. 4.3]. We put *Digits* := 200, and included enough terms of the sequence determining the eigenvector to achieve stability. For each θ it appeared that $\sigma_n(\theta)$ was an increasing function of n, so the limiting value is probably larger than the computed value. For $\theta = 0$ the operator H is self-adjoint, and the projections have norm 1. As stated earlier one must restrict θ to the range $|\theta| < \pi/4$. The results are shown for $n = 100$ in Table 1. The second column lists the constants $s_\theta^{-2} = \sec(2\theta)$ (rounded down) associated with the lower bound of Theorem 1. The fourth column lists the constants $4s_\theta^{-2} = 4\sec(2\theta)$ (rounded up) associated with the upper bound of Theorem 5. The final column lists the values of $\mu(\theta) = \exp(\tan(2\theta))$, for reasons explained below.

The approximations $\mu(\theta)$ were obtained by the following non-rigorous method. For even values of n the eigenfunction ϕ_n of H is an even function of x which is concentrated around the points $\pm x_0$, where x_0 is defined below. On the positive

θ	s_θ^{-2}	$\sigma_{100}(\theta)$	$4s_\theta^{-2}$	$\mu(\theta)$
0	1	1	4	1
0.025	1.012	1.165	4.050	1.172
0.05	1.051	1.369	4.206	1.384
0.1	1.236	1.953	4.945	2.068
0.15	1.701	3.062	6.806	3.961
0.20	3.236	6.282	12.945	21.708

Table 1

half-line the semi-classical analysis of [2, Sect. 2] suggests that for large enough $\eta > 0$

$$\phi(s+x_0) \sim \mathrm{e}^{-\psi_1 s - \psi_2 s^2/2}$$

is an approximate eigenvector of H with approximate eigenvalue λ, where $x_0 = \eta$, $\psi_1 = i\eta$, $\psi_2 = -iz^4$, and $\lambda = (1+z^4)\eta^2$; in the notation of [2] we are putting $c = z^4$ and $\alpha = 1$, and are ignoring the term involving ψ_3.

If n is a positive integer and we put $\eta = \{n/\cos(2\theta)\}^{1/2}$, then a direct calculation shows that $\lambda = 2nz^2$, which equals the nth eigenvalue of H to leading order as $n \to \infty$. This suggests that

$$\begin{aligned}
\|P_n\| &\sim \frac{\int_0^\infty |\phi(s+x_0)|^2 \, \mathrm{d}s}{|\int_0^\infty \phi(s+x_0)^2 \, \mathrm{d}s|} \\
&\sim \frac{\int_{-\infty}^\infty \mathrm{e}^{-2\mathrm{Re}\,(\psi_1)s - \mathrm{Re}\,(\psi_2)s^2} \, \mathrm{d}s}{|\int_{-\infty}^\infty \mathrm{e}^{-2\psi_1 s - \psi_2 s^2} \, \mathrm{d}s|} \\
&= \exp\{n\tan(2\theta)\}.
\end{aligned}$$

In view of the crude character of the approximations above, the similarity of $\sigma_{100}(\theta)$ and $\mu(\theta)$ in Table 1 is interesting. We conjecture that a more detailed semiclassical analysis might yield the correct asymptotic constant. This also seems the best hope for treating more general non-self-adjoint Schrödinger operators.

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